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Fast and stable evaluation of the exact absorbing boundary condition for the semi-discrete linear Schrödinger equation in unbounded domains☆

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Abstract

This paper is concerned with the numerical solution of the one-dimensional semi-discrete linear Schrödinger equation in unbounded domains. In order to compute the solution on the domain of physical interest, the artificial boundary method is applied to transform the original unbounded domain problem into an initial boundary value problem on a truncated finite domain. We prove the stability of the truncated semi-discrete problem. After that, a fast algorithm is proposed to approximate the nonlocal absorbing boundary condition. The novelty of this fast algorithm is that the stability of the approximate truncated semi-discrete problem is automatically maintained. In the end, numerical examples are presented to demonstrate the performance of the proposed algorithm.

Keywords: Absorbing boundary condition, Semi-discrete linear Schrödinger equation, Fast algorithm, Stability

1. Introduction

The Schrödinger equation plays an important role in natural science. Not only in quantum mechanics, but also in various fields such as underwater acoustics and optics, there appears the equivalent form of the Schrödinger equation, see for example [1–3]. In many cases, the Schrödinger equation is formulated on some unbounded domain, and cannot be solved analytically.

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During the past two decades, great efforts have been devoted to overcoming the difficulty arising from the unboundedness of definition domain. Among them, the artificial boundary method is one of the most popular choices.

There are various types of boundary conditions with different properties, such as nonlocal or local, explicit or implicit ones, see the monograph [4] or the review paper [5]. This paper is concerned with the implementation of nonlocal absorbing boundary conditions for the one-dimensional linear Schrödinger equation in unbounded domains. As to the designing of local boundary conditions for the Schrödinger equation, we refer the readers to the references [6–8].

In general, there are two main approaches to obtaining numerically implementable nonlocal absorbing boundary conditions, as discussed in [9]. One is to discretize the exact boundary conditions of the continuous problem, see for example, [10, 11]. For the exact boundary conditions of the continuous Schrödinger equation, we refer the readers to [12, 13]. It is known that improper discretization of the continuous boundary conditions may lead to problems such as significant spurious reflection, destruction of the unconditional stability of the interior scheme [10] and reduction of convergence rate [14]. An alternative method is to use the exact boundary conditions of the discretized Schrödinger equation. This method is relatively easier to maintain the unconditional stability of the overall scheme, and has been implemented to different types of discretization, for example, the fully discrete case in [15], temporal semi-discrete case in [16] and spatial semi-discrete case in [17].

No matter which method is employed, the derived exact boundary condition involves some convolution which is nonlocal in time. This necessitates the fast convolution algorithm, since otherwise, long time computation with a large number of time steps would be very expensive. Two fast algorithms for the Schrödinger equation have been proposed in [15] and [18], respectively. Until now, there is no stability analysis for either of them. In this paper, we aim at a novel fast algorithm whose stability can be proved rigorously, as accomplished in [19] for the one-dimensional heat equation in unbounded domains.

The rest of this paper is organized as follows. In section 2 and 3, we present our problem setting and derive the exact absorbing boundary condition for the semi-discrete Schrödinger equation. In section 4, we prove the stability of the truncated bounded domain problem. Section 5 contains the discretization of the exact nonlocal absorbing boundary conditions and the

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corresponding stability analysis. The fast algorithm is also discussed there. In the last section, we demonstrate the performance of our algorithm with several numerical examples.

2. Semi-discrete Schrödinger equation

We consider the following general semi-discrete Schrödinger equation:

$$\mathrm{i}\frac{d}{dt}q_n = a_n q_{n-1} + b_n q_n + a_{n+1}q_{n+1},\ n \in \mathbb{Z},\ t \in [0,T], \tag{2.1}$$

$$q_n(0) = c_n,\ n \in \mathbb{Z}, \tag{2.2}$$

$$q_n \to 0,\ |n| \to +\infty,\ 0 \le t \le T, \tag{2.3}$$

where $a_n = a_n(t)$ and $b_n = b_n(t)$ are smooth real-valued functions of the t-variable. We assume that the initial value c_n has compact support, the coefficients a_n and b_n become constant when the index n is suitably far away from zero. More precisely, there exists an integer $N \ge 1$ such that $c_n = 0$ as $|n| \ge N$, and

$$a_n = \begin{cases} a_r, & n \ge N, \\ a_l, & n \le -N, \end{cases} \qquad b_n = \begin{cases} b_r, & n \ge N, \\ b_l, & n \le -N. \end{cases}$$

The problem (2.1)-(2.3) may arise from a spatial discretization of the continuous Schrödinger equation, or a discrete quantum system with an infinite number of degrees of freedom.

Our goal is to develop an efficient numerical method to approximate the exact solution in a finite spatial domain. To achieve this, let us divide the spatial domain into three parts and introduce the following notations

$$\begin{aligned} \Omega_l &= \{n \in \mathbb{Z} | n \le -N\}, \\ \Omega_i &= \{n \in \mathbb{Z} | -N \le n \le N\}, \\ \Omega_r &= \{n \in \mathbb{Z} | n \ge N\}. \end{aligned}$$

In the next section, we will deduce the exact absorbing boundary conditions at the interface points $\Gamma_l = \{n = -N\}$ and $\Gamma_r = \{n = N\}$ by considering the Schrödinger equation restricted onto the exterior domains Ω_l and Ω_r.

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3. Derivation of the exact absorbing boundary condition

To obtain the boundary condition at Γ_r, let us consider the following semi-infinite Schrödinger equation:

$$\mathrm{i}\frac{d}{dt}q_n = a_r q_{n-1} + b_r q_n + a_r q_{n+1},\ n \geq N, \tag{3.1}$$

$$q_n(0) = 0,\ n \geq N+1, \tag{3.2}$$

$$q_n \to 0,\ |n| \to +\infty,\ 0 \leq t \leq T, \tag{3.3}$$

and introduce the notation

$$w_r(z) = \mathrm{i}(a_r(z + z^{-1}) + b_r). \tag{3.4}$$

We assume that a_r and b_r are prescribed to ensure the following stability condition

$$\Re w_r(z) \geq 0,\ \forall\, |z| = 1.$$

To derive the boundary condition, we begin with the z-transform of $\{q_n\}$. Let us define

$$\hat{q}(z,t) := \sum_{n=1}^{+\infty} z^{-n} q_{n+N}(t).$$

For any $z \in C\backslash\{0\}$ and $n \geq 0$, it is straightforward to verify that

$$\begin{aligned}
&\frac{d}{dt}\left[z^{-n}e^{w_r(z)t}q_{n+N}\right]\\
=&z^{-n}e^{w_r(z)t}\left[w_r(z)q_{n+N} - \mathrm{i}(a_r q_{n+N-1} + b_r q_{n+N} + a_r q_{n+N+1})\right]\\
=&-\mathrm{i}a_r z^{-n}e^{w_r(z)t}\left(q_{n+N-1} - (z+z^{-1})q_{n+N} + q_{n+N+1}\right)\\
=&-\mathrm{i}a_r z^{-(n-1)}e^{w_r(z)t}(z^{-1}q_{n+N-1} - q_{n+N})\\
&+\mathrm{i}a_r z^{-n}e^{w_r(z)t}(z^{-1}q_{n+N} - q_{n+N+1}).
\end{aligned}$$

Summing up the index n from 1 to ∞ yields

$$\frac{d}{dt}\left[e^{w_r(z)t}\hat{q}(z,t)\right] = -\mathrm{i}a_r e^{w_r(z)t}(z^{-1}q_N - q_{N+1}),\ \forall\, |z| = 1. \tag{3.5}$$

Then we obtain

$$e^{w_r(z)t}\hat{q}(z,t) = -\mathrm{i}a_r \int_0^t e^{w_r(z)\tau}\left[z^{-1}q_N(\tau) - q_{N+1}(\tau)\right]d\tau,\ \forall\, |z| = 1,$$

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which is equivalent to

$$\hat{q}(z,t) = -\mathrm{i}a_r e^{-w_r(z)t} * [z^{-1}q_N(t) - q_{N+1}(t)],\ \forall\, |z| = 1. \tag{3.6}$$

Here and hereafter, the symbol $*$ stands for the Laplace convolution operator.

According to the definition (3.4) of w_r , it holds that

$$w_r(z) = w_r(z^{-1}).$$

Therefore, recalling (3.6) we have

$$\hat{q}(z^{-1},t) = -\mathrm{i}a_r e^{-w_r(z)t} * [zq_N(t) - q_{N+1}(t)],\ \forall\, |z| = 1. \tag{3.7}$$

By subtracting (3.7) from (3.6), we deduce that

$$\hat{q}(z,t) - \hat{q}(z^{-1},t) = -\mathrm{i}a_r(z^{-1} - z)\left[e^{-w_r(z)t} * q_N(t)\right],\ \forall\, |z| = 1.$$

The function $\hat{q}(z^{-1},t)$ is analytic in the unit sphere. Thus, performing the inverse z-transform on the unit circle S^1 gives us the expression of $q_{n+N}(t)$:

$$\begin{aligned} q_{n+N}(t) &= \frac{1}{2\pi\mathrm{i}}\int_{S^1} z^{n-1}\hat{q}(z,t)dz \\ &= -\frac{a_r}{2\pi}\int_{S^1} z^{n-1}(z^{-1} - z)\left[e^{-w_r(z)t} * q_N(t)\right]dz,\ \forall\, n \geq 1. \end{aligned}$$

The above solution expression is inspired by [20, 21]. In particular, for $n = 1$ we have

$$\begin{aligned} q_{N+1}(t) &= -\frac{a_r}{2\pi}\int_{S^1}(z^{-1} - z)\left[e^{-w_r(z)t} * q_N(t)\right]dz \\ &= -\frac{\mathrm{i}a_r}{2\pi}\int_{-\pi}^{\pi}(1 - e^{2\mathrm{i}\theta})\left[e^{-w_r(e^{\mathrm{i}\theta})t} * q_N(t)\right]d\theta \\ &= -\frac{\mathrm{i}a_r}{\pi}\int_{0}^{\pi}(1 - \cos 2\theta)\left[e^{-w_r(e^{\mathrm{i}\theta})t} * q_N(t)\right]d\theta. \end{aligned} \tag{3.8}$$

The last equality holds since $w_r(e^{\mathrm{i}\theta})$ is an even function with respect to the variable θ. Introducing a new measure

$$d\nu_\theta = \frac{1}{\pi}(1 - \cos 2\theta)d\theta,$$

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we rewrite the boundary condition at Γ_r (3.8) in a more convenient form

$$q_{N+1}(t) = -\mathrm{i}a_r \int_0^\pi e^{-w_r(e^{\mathrm{i}\theta})t} * q_N(t) d\nu_\theta. \tag{3.9}$$

Similarly, we can obtain the boundary condition at Γ_l

$$q_{-N-1}(t) = -\mathrm{i}a_l \int_0^\pi e^{-w_l(e^{\mathrm{i}\theta})t} * q_{-N}(t) d\nu_\theta, \tag{3.10}$$

where

$$w_l(e^{\mathrm{i}\theta}) = \mathrm{i}(b_l + 2a_l \cos\theta).$$

4. Stability of the truncated semi-discrete Schrödinger equation

With the boundary conditions (3.9) and (3.10), the truncated problem is formulated as follows:

$$\mathrm{i}\frac{d}{dt}q_n = a_n q_{n-1} + b_n q_n + a_{n+1} q_{n+1}, \ -N \le n \le N, \ t \in [0, T], \tag{4.1}$$

$$q_n(0) = c_n, \ -N \le n \le N, \tag{4.2}$$

$$q_{N+1}(t) = -\mathrm{i}a_r \int_0^\pi e^{-w_r(e^{\mathrm{i}\theta})t} * q_N(t) d\nu_\theta, \tag{4.3}$$

$$q_{-N-1}(t) = -\mathrm{i}a_l \int_0^\pi e^{-w_l(e^{\mathrm{i}\theta})t} * q_{-N}(t) d\nu_\theta. \tag{4.4}$$

For any $\alpha > 0$, let us set $q_{n,\alpha}(t) = q_n(t)e^{-\alpha t}$. Then

$$\mathrm{i}\frac{d}{dt}q_{n,\alpha} = a_n q_{n-1,\alpha} + (b_n - \mathrm{i}\alpha)\, q_{n,\alpha} + a_{n+1} q_{n+1,\alpha}, \quad -N \le n \le N.$$

The corresponding energy is defined as follows

$$E_\alpha(t) = \sum_{n=-N}^{N} |q_{n,\alpha}(t)|^2.$$

It is straightforward to verify that for $-N \le n \le N$, it holds that

$$\frac{d}{dt}|q_{n,\alpha}|^2 = 2\Im\left[a_{n+1}\bar{q}_{n,\alpha}q_{n+1,\alpha} - a_n\bar{q}_{n-1,\alpha}q_{n,\alpha}\right] - 2\alpha|q_{n,\alpha}|^2.$$

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Summing up the above equation with respect to the index n, we arrive at

$$\begin{aligned}\frac{d}{dt}E_\alpha(t) &= \sum_{n=-N}^{N}\left\{2\Im\left[a_{n+1}\bar{q}_{n,\alpha}q_{n+1,\alpha}-a_n\bar{q}_{n-1,\alpha}q_{n,\alpha}\right]-2\alpha|q_{n,\alpha}|^2\right\}\\ &= 2\Im\left[a_{N+1}\bar{q}_{N,\alpha}q_{N+1,\alpha}-a_{-N}\bar{q}_{-N-1,\alpha}q_{-N,\alpha}\right]-2\sum_{n=-N}^{N}\alpha|q_{n,\alpha}|^2\\ &\le 2\Im[a_r\bar{q}_{N,\alpha}q_{N+1,\alpha}-a_l\bar{q}_{-N-1,\alpha}q_{-N,\alpha}],\end{aligned}\tag{4.5}$$

which leads to

$$\begin{aligned}E_\alpha(T) &\le E_\alpha(0)+2\int_0^T[\Im(a_r\bar{q}_{N,\alpha}q_{N+1,\alpha})-\Im(a_l\bar{q}_{-N-1,\alpha}q_{-N,\alpha})]dt\\ &= E_\alpha(0)+2\int_0^T[\Im(a_r\bar{q}_{N,\alpha}q_{N+1,\alpha})+\Im(a_l\bar{q}_{-N,\alpha}q_{-N-1,\alpha})]dt.\end{aligned}\tag{4.6}$$

We have noticed that the relationship between $q_{N+1,\alpha}$ and $q_{N,\alpha}$ is similar to that between $q_{-N-1,\alpha}$ and $q_{-N,\alpha}$.

Lemma 1. *Let $f(t)$ and $g(t)$ be two functions satisfying*

$$g(t)=e^{-\alpha t}\int_0^\pi e^{-w(\theta)t}*[f(t)e^{\alpha t}]d\phi_\theta,\tag{4.7}$$

where $d\phi_\theta$ is a positive measure, and $\alpha>0$ is an arbitrary constant. If $w(\theta)$ is purely imaginary for all $\theta\in[0,\pi]$, then given an arbitrary but fixed $T>0$, it holds that

$$\Re\int_0^T\bar{f}(t)g(t)dt\ge 0.$$

Proof. By a direct calculation and the Plancherel identity, we arrive at

$$\begin{aligned}\int_0^T\bar{f}(t)g(t)dt &= \int_0^T\bar{f}(t)e^{-\alpha t}\int_0^\pi e^{-w(\theta)t}*[f(t)e^{\alpha t}]d\phi_\theta dt\\ &= \int_0^\pi\int_0^T\bar{f}(t)\left[e^{-[w(\theta)+\alpha]t}*f(t)\right]dtd\phi_\theta\\ &= \int_0^\pi\int_0^\infty\overline{\chi_{[0,T]}f(t)}\left[e^{-[w(\theta)+\alpha]t}*\chi_{[0,T]}f(t)\right]dtd\phi_\theta\\ &= \frac{1}{2\pi}\int_0^\pi\int_{-\infty}^\infty\overline{\widehat{\chi_{[0,T]}f}(\mathrm{i}\xi)}\frac{\widehat{\chi_{[0,T]}f}(\mathrm{i}\xi)}{\mathrm{i}\xi+w(\theta)+\alpha}d\xi d\phi_\theta\\ &= \frac{1}{2\pi}\int_0^\pi\int_{-\infty}^\infty\left|\widehat{\chi_{[0,T]}f}(\mathrm{i}\xi)\right|^2\frac{1}{\mathrm{i}\xi+w(\theta)+\alpha}d\xi d\phi_\theta.\end{aligned}$$

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Since $w(\theta)$ is purely imaginary and $\alpha > 0$, the real part of $1/[\mathrm{i}\xi + w(\theta) + \alpha]$ is positive. The proof thus ends by taking the real part of the above equation.

Therefore, by applying Lemma 1 to $q_{N+1,\alpha}$ and $q_{N,\alpha}$, we arrive at

$$\begin{aligned} &\Im\left[a_r \int_0^T \bar{q}_{N,\alpha} q_{N+1,\alpha} dt\right] \\ =&\Im\left[-\mathrm{i}a_r^2 \int_0^T \bar{q}_{N,\alpha} e^{-\alpha t} \int_0^\pi e^{-w_r(e^{\mathrm{i}\theta})t} * q_N(t) d\nu_\theta dt\right] \\ =&-\Re\left[a_r^2 \int_0^T \bar{q}_{N,\alpha} e^{-\alpha t} \int_0^\pi e^{-w_r(e^{\mathrm{i}\theta})t} * [q_{N,\alpha}(t) e^{\alpha t}] d\nu_\theta dt\right] \leq 0. \end{aligned} \tag{4.8}$$

Similar result holds for the second part of integrant in (4.6):

$$\Im\left[a_l \int_0^T \bar{q}_{-N,\alpha} q_{-N-1,\alpha} dt\right] \leq 0. \tag{4.9}$$

Substituting (4.8) and (4.9) into (4.6), we arrive at

$$E_\alpha(T) \leq E_\alpha(0),\ T > 0,\ \alpha > 0.$$

Taking the limit of the above expression as α approaches zero, we obtain the following stability result for the truncated problem (4.1)-(4.4).

Theorem 2. *The semi-infinite ODE system (4.1)-(4.4) is stable. More precisely, let us put*

$$E(t) = \sum_{n=-N}^{N} |q_n(t)|^2. \tag{4.10}$$

Then it holds that

$$E(T) \leq E(0),\ \forall\, T > 0.$$

5. Fast algorithm, stability and error estimate

In the numerical implementation, the integrals involved in the exact boundary condition (4.3) and (4.4) should be discretized by some quadrature rule. Let us set

$$\theta_m = \frac{2m-1}{2M}\pi,\ \forall\, m = 1, \ldots, M,$$

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where M is a prescribed positive integer. Applying the composite midpoint quadrature rule with equidistant step length π/M, we derive two approximate boundary conditions

$$q_{N+1}(t) = -\mathrm{i}a_r \int_0^\pi \left[e^{-w_r(e^{\mathrm{i}\theta})t} * q_N(t) \right] d\mu_\theta, \tag{5.1}$$

$$q_{-N-1}(t) = -\mathrm{i}a_l \int_0^\pi \left[e^{-w_l(e^{\mathrm{i}\theta})t} * q_{-N}(t) \right] d\mu_\theta, \tag{5.2}$$

where μ_θ is the discrete measure

$$d\mu_\theta = \sum_{m=1}^{M} \frac{(1-\cos 2\theta_m)}{M} \delta(\theta - \theta_m) d\theta.$$

Replacing the exact boundary conditions (4.3) and (4.4) with the above discrete boundary conditions, we derive the following approximate semi-infinite ODE system:

$$\mathrm{i}\frac{d}{dt}q_n = a_n q_{n-1} + b_n q_n + a_{n+1} q_{n+1}, \ -N \le n \le N, \ t \in [0,T], \tag{5.3}$$

$$q_n(0) = c_n, \ -N \le n \le N, \tag{5.4}$$

$$q_{N+1}(t) = -\mathrm{i}a_r \int_0^\pi \left[e^{-w_r(e^{\mathrm{i}\theta})t} * q_N(t) \right] d\mu_\theta, \tag{5.5}$$

$$q_{-N-1}(t) = -\mathrm{i}a_l \int_0^\pi \left[e^{-w_l(e^{\mathrm{i}\theta})t} * q_{-N}(t) \right] d\mu_\theta. \tag{5.6}$$

For fast algorithm of the convolution, let us introduce

$$\mathcal{G}_{r,m}(t) = e^{-w_r(e^{\mathrm{i}\theta_m})t} * q_N(t), \ m = 1, \cdots, M,$$
$$\mathcal{G}_{l,m}(t) = e^{-w_l(e^{\mathrm{i}\theta_m})t} * q_{-N}(t), \ m = 1, \cdots, M.$$

Then $\mathcal{G}_{k,m}$ with $k \in \{l, r\}$ and $m \in [1, M]$ satisfies the following initial value problem

$$\frac{d}{dt}\mathcal{G}_{r,m}(t) = -w_r(e^{\mathrm{i}\theta_m})\mathcal{G}_{r,m}(t) + q_N(t),$$
$$\frac{d}{dt}\mathcal{G}_{l,m}(t) = -w_l(e^{\mathrm{i}\theta_m})\mathcal{G}_{l,m}(t) + q_{-N}(t),$$
$$\mathcal{G}_{r,m}(0) = 0,$$
$$\mathcal{G}_{l,m}(0) = 0.$$

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Therefore, the ODE system (5.3)-(5.6) is equivalent to the following augmented ODE system:

$$
\begin{aligned}
&\mathrm{i}\frac{d}{dt}q_N = a_N q_{N-1} + b_N q_N + a_{N+1}\left[-\frac{\mathrm{i}a_r}{M}\sum_{m=1}^{M}(1-\cos 2\theta_m)\mathcal{G}_{r,m}(t)\right],\\
&\mathrm{i}\frac{d}{dt}q_n = a_n q_{n-1} + b_n q_n + a_{n+1}q_{n+1},\ -N+1 \le n \le N-1,\\
&\mathrm{i}\frac{d}{dt}q_{-N} = a_{-N+1} q_{-N+1} + b_{-N} q_{-N} + a_{-N}\left[-\frac{\mathrm{i}a_l}{M}\sum_{m=1}^{M}(1-\cos 2\theta_m)\mathcal{G}_{l,m}(t)\right],\\
&\frac{d}{dt}\mathcal{G}_{r,m}(t) = -w_r(e^{\mathrm{i}\theta_m})\mathcal{G}_{r,m}(t) + q_N(t),\ 1 \le m \le M,\\
&\frac{d}{dt}\mathcal{G}_{l,m}(t) = -w_l(e^{\mathrm{i}\theta_m})\mathcal{G}_{l,m}(t) + q_{-N}(t),\ 1 \le m \le M,\\
&q_n(0) = c_n,\ -N \le n \le N,\\
&\mathcal{G}_{r,m}(0) = 0,\ 1 \le m \le M,\\
&\mathcal{G}_{l,m}(0) = 0,\ 1 \le m \le M.
\end{aligned}
$$

We can apply a suitable ODE solver to directly solve the above system, instead of computing the convolutions involved in (5.3)-(5.6). Next, we prove the stability of the approximate problem (5.3)-(5.6).

Theorem 3. *The ODE system (5.3)-(5.6) is stable under the perturbation of the initial data and boundary conditions. More precisely, suppose q_n is a solution of the following problem*

$$
\begin{aligned}
&\mathrm{i}\frac{d}{dt}q_n = a_n q_{n-1} + b_n q_n + a_{n+1}q_{n+1},\ -N \le n \le N,\ t \in [0,T],\\
&q_n(0) = c_n,\ -N \le n \le N,\\
&q_{N+1}(t) = -\mathrm{i}a_r\int_0^{\pi}\left[e^{-w_r(e^{\mathrm{i}\theta})t} * q_N(t)\right]d\mu_\theta + \epsilon_r(t),\\
&q_{-N-1}(t) = -\mathrm{i}a_l\int_0^{\pi}\left[e^{-w_l(e^{\mathrm{i}\theta})t} * q_{-N}(t)\right]d\mu_\theta + \epsilon_l(t),
\end{aligned}
\tag{5.7}
$$

where ϵ_r and ϵ_l are two functions of t satisfying

$$\max_{i\in\{r,l\}}\sup_{t\in[0,T]}|\epsilon_i(t)| < \epsilon < \infty.$$

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Then for an arbitrary but fixed $T > 0$, it holds that

$$\sup_{t\in[0,T]} E(t) \le C\left[E(0) + \epsilon^2\right],$$

where C is a constant depending on T and $E(t)$ is defined in (4.10).

Proof. Let us recall the following notations

$$q_{n,\alpha}(t) = q_n(t)e^{-\alpha t},\ \alpha > 0,$$
$$E_\alpha(t) = \sum_{n=-N}^{N} |q_{n,\alpha}(t)|^2.$$

Analogous to (4.5), we have

$$\begin{aligned}\frac{d}{dt}E_\alpha(t) &\le 2\Im[a_r\bar{q}_{N,\alpha}q_{N+1,\alpha} - a_l\bar{q}_{-N-1,\alpha}q_{-N,\alpha}]\\ &= 2\Im[a_r\bar{q}_{N,\alpha}q_{N+1,\alpha} + a_l\bar{q}_{-N,\alpha}q_{-N-1,\alpha}]\end{aligned} \tag{5.8}$$

Since

$$\begin{aligned}a_r\bar{q}_{N,\alpha}q_{N+1,\alpha} &= -\mathrm{i}a_r^2K_r + a_r\epsilon_r e^{-\alpha t}\bar{q}_{N,\alpha},\\ a_l\bar{q}_{-N,\alpha}q_{-N-1,\alpha} &= -\mathrm{i}a_l^2K_l + a_l\epsilon_l e^{-\alpha t}\bar{q}_{-N,\alpha},\end{aligned}$$

where we have set

$$\begin{aligned}K_r(t) &= e^{-\alpha t}\bar{q}_{N,\alpha}\int_0^\pi e^{-w_r(e^{\mathrm{i}\theta})t} * [q_{N,\alpha}(t)e^{\alpha t}]d\mu_\theta,\\ K_l(t) &= e^{-\alpha t}\bar{q}_{-N,\alpha}\int_0^\pi e^{-w_l(e^{\mathrm{i}\theta})t} * [q_{-N,\alpha}(t)e^{\alpha t}]d\mu_\theta,\end{aligned}$$

from (5.8), it holds that

$$\begin{aligned}\frac{d}{dt}E_\alpha(t) \le& -2\Re(a_r^2K_r + a_l^2K_l) + 2a_re^{-\alpha t}\Im(\epsilon_r\bar{q}_{N,\alpha}) + 2a_le^{-\alpha t}\Im(\epsilon_l\bar{q}_{-N,\alpha})\\ \le& -2\Re(a_r^2K_r + a_l^2K_l) + 2\epsilon a_re^{-\alpha t}|\bar{q}_{N,\alpha}| + 2\epsilon a_le^{-\alpha t}|\bar{q}_{-N,\alpha}|\\ \le& -2\Re(a_r^2K_r + a_l^2K_l) + E_\alpha(t) + \epsilon^2[(a_r)^2 + (a_l)^2]e^{-2\alpha t}.\end{aligned}$$

Integrating the above inequality with respect to t and applying Lemma 1 to K_r and K_l on the right hand side, we arrive at

$$E_\alpha(t) - E_\alpha(0) \le \int_0^t E_\alpha(\tau)d\tau + \frac{\epsilon^2(1-e^{-2\alpha t})}{2\alpha}[(a_r)^2 + (a_l)^2].$$

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Applying Gronwall's inequality yields

$$E_\alpha(t) \le e^t \left\{ E_\alpha(0) + \frac{\epsilon^2(1-e^{-2\alpha t})}{2\alpha}[(a_r)^2 + (a_l)^2] \right\}.$$

Taking the limit of the above expression as α approaches zero, we finish the proof by setting

$$C = e^T \max\{1, T(a_r^2 + a_l^2)\}.$$

We are now ready to estimate the error between the solution of problem (5.3)-(5.6) and that of problem (4.1)-(4.4).

Theorem 4. *Let q_n be the solution of the approximate truncated problem (5.3)-(5.6) and Q_n be the solution of the exact truncated problem (4.1)-(4.4). Set $e_n = q_n - Q_n$. Then for an arbitrary but fixed $T > 0$, it holds that*

$$\sup_{t\in[0,T]} \sum_{n=-N}^{N} |e_n(t)|^2 \le C\epsilon^2,$$

where

$$\epsilon = 2^{2-2M}\pi \max\{e^{2|a_l|T}\|Q_{-N}\|_{L^\infty[0,T]}, e^{2|a_r|T}\|Q_N\|_{L^\infty[0,T]}\},$$

and C is a constant depending on T.

Proof. It is straightforward to verify that the error function $e_n = e_n(t)$ satisfies the following problem

$$\begin{aligned}
&\mathrm{i}\frac{d}{dt}e_n(t) = a_n e_{n-1}(t) + b_n e_n(t) + a_{n+1}e_{n+1}(t),\ -N \le n \le N,\ t \in [0,T],\\
&e_n(0) = 0,\ -N \le n \le N,\\
&e_{N+1}(t) = -\mathrm{i}a_r \int_0^\pi e^{-w_r(e^{\mathrm{i}\theta})t} * e_N(t) d\mu_\theta + \epsilon_r(t),\\
&e_{-N-1}(t) = -\mathrm{i}a_l \int_0^\pi e^{-w_l(e^{\mathrm{i}\theta})t} * e_{-N}(t) d\mu_\theta + \epsilon_l(t),
\end{aligned}$$

where

$$\begin{aligned}
\epsilon_r(t) &= -\mathrm{i}a_r \int_0^\pi \left[e^{-w_r(e^{\mathrm{i}\theta})t} * Q_N(t)\right](d\mu_\theta - d\nu_\theta),\\
\epsilon_l(t) &= -\mathrm{i}a_l \int_0^\pi \left[e^{-w_l(e^{\mathrm{i}\theta})t} * Q_{-N}(t)\right](d\mu_\theta - d\nu_\theta).
\end{aligned}$$

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To analyze $\epsilon_r(t)$, let us introduce the notation

$$E_M(f) = \int_{-1}^{1} \frac{f(x)dx}{\sqrt{1-x^2}} - \sum_{m=1}^{M} \mu_i f(x_m),$$

where $x_m = \cos[\frac{(2m-1)\pi}{2M}]$ and $\mu_m = \pi/M$. Noticing that

$$\begin{aligned}
&\int_0^{\pi} \left[e^{-w_r(e^{\mathrm{i}\theta})t} * Q_N(t)\right] d\nu_\theta \\
=&\int_0^{\pi} \frac{(1-\cos 2\theta)}{\pi} \left[e^{-\mathrm{i}(b_r+2a_r\cos\theta)t} * Q_N(t)\right] d\theta \\
=&\int_{-1}^{1} \frac{g(x)}{\sqrt{1-x^2}} dx,
\end{aligned}$$

where

$$g(x,t) = \pi^{-1}(2-2x^2)[e^{\mathrm{i}(-b_r+2a_r x)t} * Q_N(t)], \tag{5.9}$$

we have

$$\epsilon_r(t) = \mathrm{i}a_r E_M(g(\cdot,t)).$$

Since $g(\cdot,t)$ satisfies

$$\begin{aligned}
\max_{|z|=1} |g(z,t)| &= \max_{|z|=1} \left|(2-2z^2)[e^{-\mathrm{i}(b_r+2a_r z)t} * Q_N(t)]\right| \\
&\le 4 \ \|Q_N\|_{L^\infty[0,t]} \int_0^t e^{2|a_r|\tau} d\tau \\
&\le 2|a_r|^{-1} \ \|Q_N\|_{L^\infty[0,t]} e^{2|a_r|t},
\end{aligned}$$

applying Theorem 5 in the appendix with $R = 1$ yields

$$|\epsilon_r(t)| \le \pi 2^{2-2M} \|Q_N\| e^{2|a_r|T}.$$

Analogously, we have

$$|\epsilon_l(t)| \le \pi 2^{2-2M} \|Q_{-N}\| e^{2|a_l|T}.$$

By Theorem 3, we arrive at

$$\sup_{t\in[0,T]} \sum_{n=-N}^{N} |e_n(t)|^2 \le C\epsilon^2,$$

where C is a constant depending on T.

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6. Numerical examples

In this section, we present two numerical examples to demonstrate the performance of our proposed fast evaluation algorithm for the exact nonlocal absorbing boundary conditions. The approximate truncated problem (5.3)-(5.6) is integrated out simply by the MATLAB subroutine ODE45.

Example 1. We consider the semi-discrete Schrödinger equation:

$$\begin{aligned} &\mathrm{i}\frac{d}{dt}q_n = -q_{n-1} + 2q_n - q_{n+1},\ t \in [0,T], \\ &q_n(0) = \exp\left(\mathrm{i}n - \frac{n^2}{100}\right),\ n \in \mathbb{Z}. \end{aligned}$$

This example corresponds to $a_n = -1$ and $b_n = 2$ in (2.1).

Considering a Gaussian function which decays extremely fast as our initial data, we introduce an interval $[-N, N]$ and approximate the initial data on $\mathbb{Z}\backslash[-N, N]$ by zero. Then we apply the artificial boundary method and the proposed fast algorithm to compute the solution in $[-N, N]$. To quantify the influence of the initial data treatment, we list the maximum errors confined into the interval $[-30, 30]$ at $t = 10$ between the approximate solutions and the reference solution in Table 1. The reference solution is obtained by setting $N = 100$ and $M = 80$. It can be seen that the error becomes extremely small when N is suitably large. This numerical evidence not only justifies the initial data treatment, but also validates the accuracy of fast algorithm.

Table 1: maximum error in domain [-30,30] at t = 10

N	30	40	50	60	70
error	2.6×10^{-5}	1.8×10^{-8}	6.7×10^{-13}	1.2×10^{-16}	2.4×10^{-25}

Example 2. In this example, we consider the free Schrödinger equation

$$\begin{aligned} &\mathrm{i}\epsilon q_t(x,t) = -\frac{\epsilon^2}{2} q_{xx}(x,t), \\ &q(x,0) = \exp(-10x^2)\exp(1.5\mathrm{i}x/\epsilon), \end{aligned}$$

where $\epsilon = 0.01$. The exact solution of this problem is

$$q(x,t) = \frac{1}{\sqrt{1+20\mathrm{i}\epsilon t}} \exp\left[\frac{-\mathrm{i}}{2\epsilon t}\left(\frac{(1.5t-x)^2}{1+20\mathrm{i}\epsilon t} - x^2\right)\right].$$

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Given an positive integer N, we derive a semi-discrete system by approximating the second-order spatial derivative with the central difference scheme. The step length is set as $h = 1/N$. Corresponding to the frame equation (2.1), we have

$$a_n = -\frac{\epsilon}{2h^2}, \quad b_n = \frac{\epsilon}{h^2}.$$

The artificial boundary points are set at $\pm N$. We apply the artificial boundary method and the proposed fast algorithm. To figure out the influence of the number of quadrature points M, we compute the numerical solutions and compare them with a reference solution by setting $M = 400$. The maximum errors are plotted in Fig. 1. We see that these errors decay extremely fast with the increasing of M. This observation is consistent with our theoretical analysis performed in Theorem 4.

We plot the numerical solution in the left of Fig. 2. No spurious reflection can be detected. In the right of Fig. 2, we plot the errors between the numerical solutions and the exact solution. A second order convergence rate can be seen obviously.

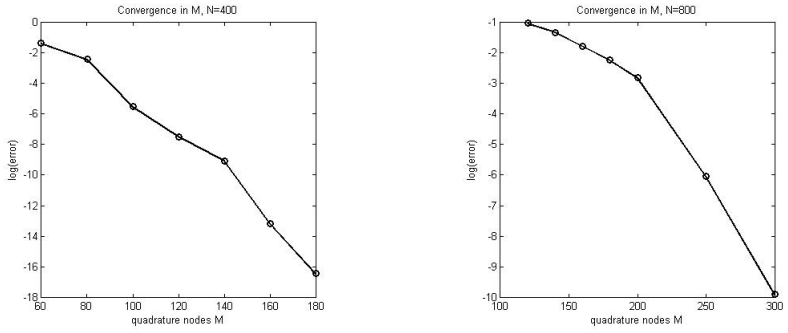


Figure 1: Example 2. Spectral accuracy with respect to the number of poles M.

7. Conclusion

This paper considered the one-dimensional semi-discrete linear Schrödinger equation in unbounded domains. We applied the artificial boundary method to transform the unbounded domain problem into a finite domain problem.

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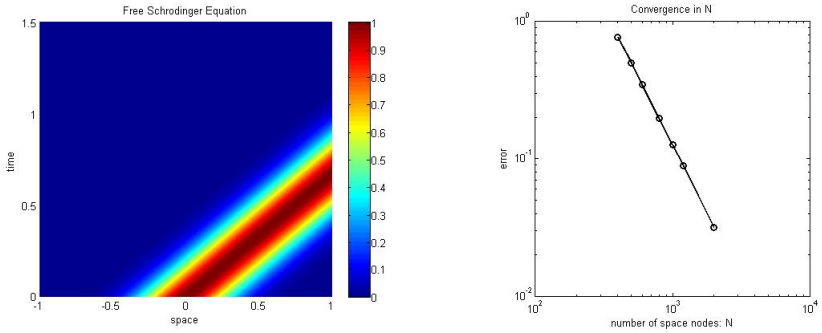


Figure 2: Example 2. The second order convergence of the maximum error in time interval $[0, 0.6]$. For $N = 400, 500, 600, 800, 1000$ and 1200, we set the number of poles $M = 400$. For $N = 2000$, we set the number of poles $M = 800$.

The exact absorbing boundary condition was derived, and a stable fast algorithm was developed. Numerical examples showed that our algorithm admits spectral accuracy with respect to the number of poles. These poles relate to the quadrature nodes used to approximate the continuous integral involved in the exact nonlocal boundary condition.

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Appendix

We list the error estimate of the Gauss-Chebyshev quadrature rule. Its proof was given by Chawla and Jain in [22].

Theorem 5. *Given a single valued function $f(z)$. Suppose it is analytic in the disk of radius R which contains the interval $[-1, 1]$. Let us define*

$$E_M(f) = \int_{-1}^{1} \frac{f(x)dx}{\sqrt{1-x^2}} - \sum_{m=1}^{M} \mu_i f(x_m),$$

where $x_m = \cos[\frac{(2m-1)\pi}{2M}]$ and $\mu_m = \pi/M$. Then

$$\left|E_M(f)\right| \leq \frac{\pi T(R)}{2^{2M-1}R^{2M}},$$

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where

$$T(R) = \max_{|z|=R} |f(z)|.$$

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